MONTE-CARLO SIMULATION OF ULTRASONIC GRAIN NOISE

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INTRODUCTION

In ultrasonic inspections for small or subtle defects in metals, defect signals may be obscured by grain noise echoes which arise from the scattering of sound by the microstructure of the metal. Models for predicting microstructural noise levels are consequently essential for accurately assessing the reliability of the ultrasonic inspections. Existing noise models, like the independent scatterer model (ISM) [1], are capable of predicting only average noise characteristics, such as the root-mean-square (rms) noise level. Average noise levels, although useful, are not sufficient for assessing detection reliability. One needs to know the manner in which noise signals are distributed about their average level. The expected peak noise level, for example, effects the rate of "false calls", in which noise signals are mistaken for echoes from critical defects. In this work, we present a Monte-Carlo method for simulating time-domain noise signals observed in pulse/echo immersion inspections of metal components. The method predicts simulated time-domain noise signals, and hence can be used to determine both average and peak noise levels. We assume that the backscattered noise is dominated by the single-scattering of the incident beam by individual metal grains. The metal volume is represented as an ensemble of spherical, single-crystal grains whose centers and orientations are randomly chosen. Grain radii are determined by the nearest-neighbor distances and volume conservation. The backscattered voltage signal from each grain is calculated by treating the grain as an anisotropic scatterer in the homogeneous average medium formed by the other grains. Backscattered signals from all grains are summed to determine the total noise signal. Calculations are then repeated for many different grain ensembles to assess average and peak noise levels. Predictions of the Monte-Carlo model are compared to experiment, and to the predictions of ISM. At a fixed time after the front-surface echo, the distribution of noise voltages about their mean value is found to become normally distributed as the density of grains increases. This is demonstrated by a series of calculations for α-phase titanium specimens with different grain densities.

NOISE CALCULATIONS

Grain noise refers to ultrasonic echoes which arise from scattering of waves by the microstructure of a metal specimen. Fig. 1. shows the normal incidence inspection of a metal specimen in pulse/echo mode in an immersion setting. We employ a time coordinate system in which the center of the front-surface echo appears at t=0. In this system, we designate a "time window of interest" (TWOI) for which our noise calculation will be

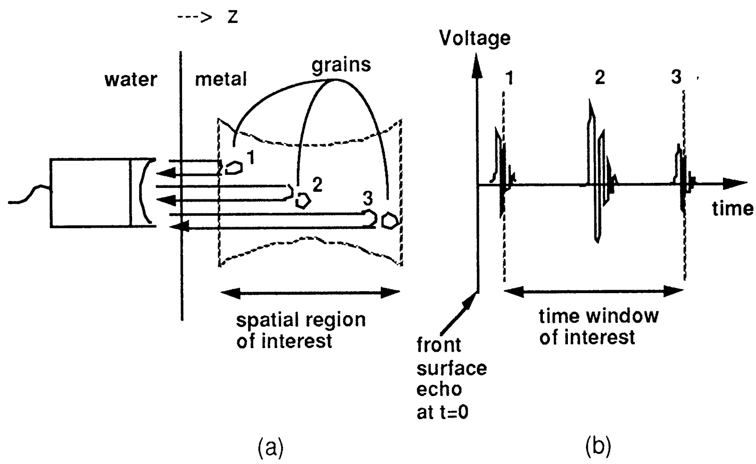

Fig. 1. (a): Geometry of ultrasonic inspection. (b): Noise voltage response.

valid. Associated with TWOI is a corresponding "spatial region of interest" (SROI) which encloses all metal grains that can produce appreciable backscattered signals in the TWOI. The minimum and maximum z-coordinates of the SROI are determined by the limits of the TWOI and the duration of the ultrasonic pulse. The lateral "envelope" of the SROI is determined by the beam profile, i.e., by the volume in which the incident field strength is appreciable. The particulars of the pulse/echo inspection which must be specified for the grain noise simulations are the time window of interest, the transducer radius and focal length, waterpath, and the material properties of the metal (density, soundspeed, attenuation, number of grains per cubic centimeter, and elastic constants for single crystals). In addition one inputs a front surface "reference" echo which serves to encode the gain settings of the pulser/receiver and the transducer efficiency. Using the ultrasonic measurement model of Thompson and Gray [2], the Fourier transform of this time-domain reference signal may be written as:

$$R(\omega) = \beta R_{00} D(\omega) \exp(-2ik_0 z_{0R} - 2\alpha_0 z_{0R}) \tag{1}$$

Using the same citation, the Fourier transform of the voltage signal observed in the noise measurement geometry due to direct scattering by a single anisotropic grain located at position (x,y,z) in the solid is:

$$\delta S(\omega,x,y,z) = [\{2\beta A(\omega)\rho_1 v_1\}/(ik_1 a^2 \rho_0 v_0)] T_{01}{}^2 C^2(\omega,x,y,z)$$
$$\exp[-2i(k_0 z_{0S} + k_1 z_{1S}) - 2(\alpha_0 z_{0S} + \alpha_1 z_{1S})] \tag{2}$$

In Eqs. (1) and (2), the host metal is treated as an attenuative isotropic medium. The symbols v, k, ρ, α, and a denote the longitudinal wave velocity, wavenumber ($k = \omega/v$), density, attenuation constant, and transducer radius, respectively. Subscripts 0 and 1 refer to water and metal, respectively and subscripts R and S refer to the reference and noise geometries which may have different waterpaths. β is the transducer efficiency. R_{00} and T_{01} are the reflection and transmission coefficients. $C(\omega,x,y,z)$ is a measure of the incident ultrasonic field strength in the metal. $D(\omega)$ accounts for the effects of diffraction losses in the reference signal. The waterpath (z_{0R} or z_{0S}) is measured outward from the transducer face along the central ray direction. Finally, $A(\omega)$ is the scattering amplitude for backscattered sound from the grain in question. The backscattering amplitude of a single grain illuminated by a longitudinal plane wave is deduced using the Born approximation [3]:

$$A(\omega) = (k^2/4\pi)\ [\ (\delta\rho/\rho) + (k^2/\rho\omega^2)\ \delta C_{33}]\ S(k) \tag{3}$$

where $\delta\rho = \rho_{grain} - \rho_{host}$ and $\delta C_{33} = (C_{33})_{grain} - (\lambda+2\mu)_{host}$

In Eq. (3), S(k) is a frequency dependent "shape factor" determined by the size and shape of the scatterer. In the present work, all grains will be assumed to be spherical. For a sphere of a radius r, the shape factor may be derived resulting in the following expression:

$$S(k,r) = 4\pi r^3\ [\ \sin(2rk) - (2rk)\ \cos(2rk)\ ]/\ (2rk)^3 \tag{4}$$

In the Monte-Carlo formulation, the spatial region of interest is filled with spherical single-crystal grains, with the total number of grains determined by the grain density (n) and the volume of the SROI. The grain centers, (x,y,z), are chosen randomly within this volume. The orientation of the principal crystalline axes of each grain are also chosen randomly from a specified distribution. The assigned radius of each grain is proportional to the distance to the center of the nearest neighboring grain, with the constant of proportionality chosen to conserve volume. The total noise signal is taken to be the simple sum of the backscattered noise echoes from each grain in SROI. Examples of three such echoes may be seen in Fig. 1b. These individual echoes are calculated using Eqs. (1)-(4). Since the reference signal is assumed to be known, Eq. (1) can be used to determine the transducer efficiency $\beta(\omega)$. For computational simplicity, the Gaussian beam model [4] is used to calculate $C(\omega,x,y,z)$. The individual noise echoes are summed in the frequency domain, and an inverse Fourier transform is then used to obtain the time-domain total noise signal. To complete the calculational algorithm, the method for determining $\delta\rho$ and δC_{33} must be specified. In the present work we restrict attention to equi-axed, single-phase cubic or hexagonal crystallites.

The elastic constants of the isotropic, macroscopic specimen are taken to be the Voigt average of the elastic constants of the individual crystallites. These are the mean isotropic stiffnesses "under constancy of strain". Average elastic properties for equiaxial distributions of crystals of hexagonal and cubic symmetry are available [5,6]. In particular:

$$(\lambda+2\mu)_{Voigt} = (8C_{11} + 3C_{33} + 4C_{13} + 8C_{44})\ /\ 15 \quad , \quad \text{hexagonal symmetry} \tag{5}$$

$$(\lambda+2\mu)_{Voigt} = (3C_{11} + 4C_{12} + 4C_{44})\ /\ 5 \quad , \quad \text{cubic symmetry} \tag{6}$$

where the C_{ij} denote the single crystal constants in a principal axis coordinate system. For each grain in SROI, three randomly chosen Euler angles, (ψ,θ,ϕ) [7] are used to orient the principal axes of the grain with respect to the lab coordinate system which is attached to the macroscopic specimen. In the lab system, the 33 components of grains stiffness matrix can be shown to be:

$$(C_{33})_{grain} = C_{11} + 2(-C_{11}+C_{13}+2C_{44})\cos^2\theta$$
$$+ (C_{11}-2C_{13}+C_{33}-4C_{44})\cos^4\theta \quad , \quad \text{hexagonal symmetry} \tag{7}$$

$$(C_{33})_{grain} = [(\sin^4\phi+\cos^4\phi)\sin^4\theta+\cos^4\theta]C_{11}$$

$$+ [2\sin^2\theta(\sin^2\phi\cos^2\phi\sin^2\theta+\cos^2\theta)](C_{12}+2C_{44}) \quad , \quad \text{cubic symmetry} \quad (8)$$

In summary, δC_{33} in Eq. (3) is evaluated for each grain using Eqs. (5)-(8). We also assume that the macroscopic specimen has the same density as each crystallite, i.e., $\delta\rho=0$.

As an example of a Monte-Carlo calculation, consider an equi-axed, α-titanium specimen with hexagonal crystallites ensonified by a 15-MHz toneburst pulse using a focused transducer having a radius of 0.607 cm and a focal length of 9.64 cm. Grains with a density of 1,000 per cubic cm are chosen to fill out the SROI which contains the focal region and occupies a volume of 0.502 cm^3. Fig 2a. shows the backscattered signal from a single grain located in the portion of the SROI nearest the transducer. The total noise signal from all 502 grains in the SROI is shown in Fig. 2b. The particular collection of 502 grains is referred to as "one ensemble" of grains, and corresponds to one transducer position in a scan pattern. By repeating the calculations for many ensembles of grains, we can estimate some quantities of interest such as the average and the peak noise levels that would be observed during an inspection. Two such quantities used throughout this paper are: the root-mean-squared average noise level seen at time t (averaged over ensembles); and the ratio of the peak noise seen at time t for any ensemble to the rms average noise at time t.

It should be re-emphasized that only those grains are included which would contribute to the noise within the TWOI. Noise signals are seen outside this window, but some grains which could contribute signals at those times have not been included.

COMPARISON WITH EXPERIMENT

It is illuminating to compare the predictions of the Monte-Carlo noise model to experimental noise measurements. In order to do this, the noise model requires the number of grains per cubic cm, n, as an input. To estimate n, one can analyze a micrograph showing the grain structure of the test specimen. The probability that a line segment of length L placed on the photo has both ends inside of one grain is next determined for the test specimen. This is then compared to the analytical expression for this

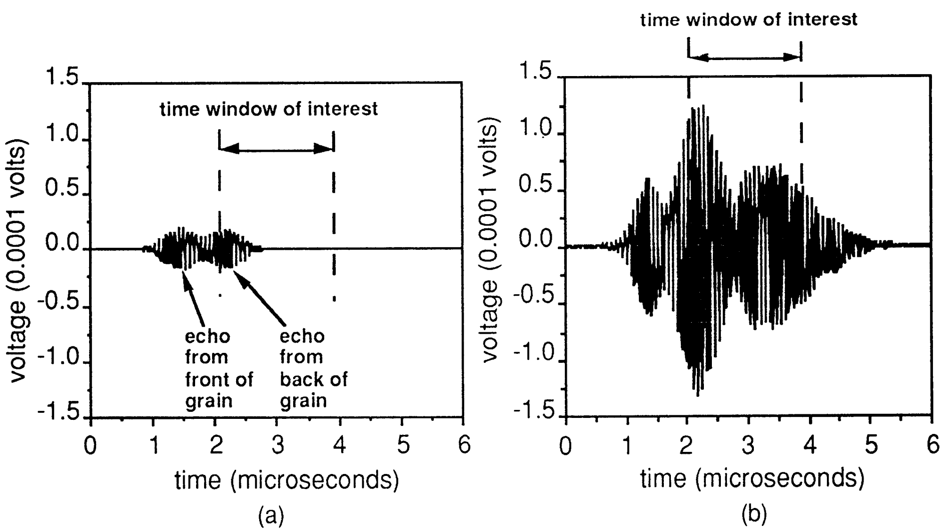

Fig. 2. Noise signals. (a): Single grain. (b) One ensemble of grains.

probability which is predicted by the Monte-Carlo calculaions as described below. One begins by determining the size distribution function of the spherical grains. If there are n grains per unit volume, the probability that a given grain has a radius between r and r+dr is found to be:

$$p(r)\ dr = 4\pi n r^2\ \exp(-4\pi n r^3/3)\ dr \tag{9}$$

Then, the probability that a line segment of length L has both ends inside of one grain may be calculated, with the result:

$$P(L) = \exp(-\pi n L^3/6) - (\pi n L^3/6)^{1/3}\ \Gamma(2/3\ ,\ 2\pi n L^3/3) \tag{10}$$

where Γ denotes the incomplete gamma function. To test this procedure, P(L) was estimated from a micrograph of an equi-axed copper specimen (cubic crystallites). By comparing with the experimental P(L) values for various grain densities of the spherical grain model, as shown in Fig. 3., we observed that a density of 100,000 grains per cubic cm was a reasonable choice.

The noise model also requires an effective ultrasonic attenuation as an input. This was estimated in two ways: the traditional analysis of multiple back surface echoes resulted in an attenuation of $\alpha = 0.01f^{2.5}$ nepers per cm for 1 MHz<f<8 MHz; and the analysis of backscattered noise as a function of depth resulted in an attenuation of $\alpha = 0.05f^{1.2}$ nepers per cm for 2 MHz<f<6 MHz. Both attenuations were used in subsequent model noise calculations.

The specimen was ensonified by a 5-MHz broadband pulse using a focused transducer having a radius of 0.636 cm and a focal length of 7.2 cm. Backscattered noise echoes were obtained at 100 transducer positions. The measured rms average noise level is shown in Fig. 4a., and compared with model predictions for 100 ensembles for each of the two attenuation functions. In this case, the SROI brackets the focal zone which is centered 0.7

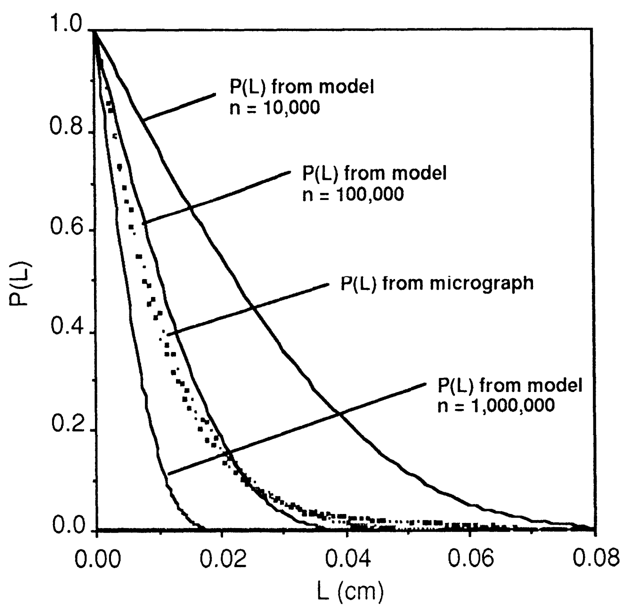

Fig. 3. The probability distribution function of a line segment placed on microstructure.

cm beneath the front surface. Fig. 4b. shows the ratio of the peak noise to the rms noise seen in the experiment and predicted by the model. Measured and predicted noise characteristics are seen to be in good agreement. Note that the predicted absolute noise signals are about 70 dB below the input front surface reference signal, and no adjustable parameters are involved in the noise calculations.

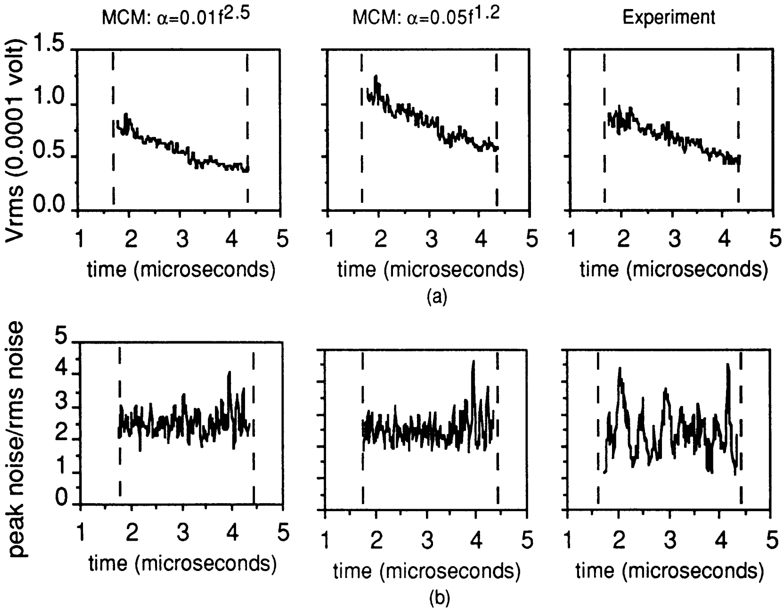

Fig. 4. Noise signals from Copper. (a): RMS noise levels. (b): Peak to rms noise levels.

MODEL APPLICATIONS

One use of the Monte-Carlo model is to test other single-scattering models and techniques for noise signal analysis. The independent scatterer model (ISM), for example, predicts the rms average noise level from the measurement system parameters and the microstructural quantity $n^{1/2}|A|_{rms}$ which is known as the "figure-of-merit" (FOM) [1,8]. In the following example, we predict backscattered noise from an α-phase titanium specimen ensonified with a 15-MHz toneburst from a focused transducer (a=0.607 cm and F=9.65 cm). The rms noise levels near the focal zone are predicted for seven different grain densities for both the Monte-Carlo and the independent scatterer models as shown in Fig. 5. The Monte-Carlo results employ 500 ensembles for each density. Although, the average noise levels are seen in Fig. 5. to increase with increasing grain density, the rms noise level is expected to drop with further increase in grain density at some point.

The Monte-Carlo noise model may also be used to determine how noise voltages are distributed about their mean value. We have determined the probability distribution of noise voltages for the aforementioned α-titanium inspection. This was done by constructing a histogram of all noise voltages seen for all ensembles in a short-duration time window. Results for a low and a high density of grains are shown in Figs. 6a. and 6b.,

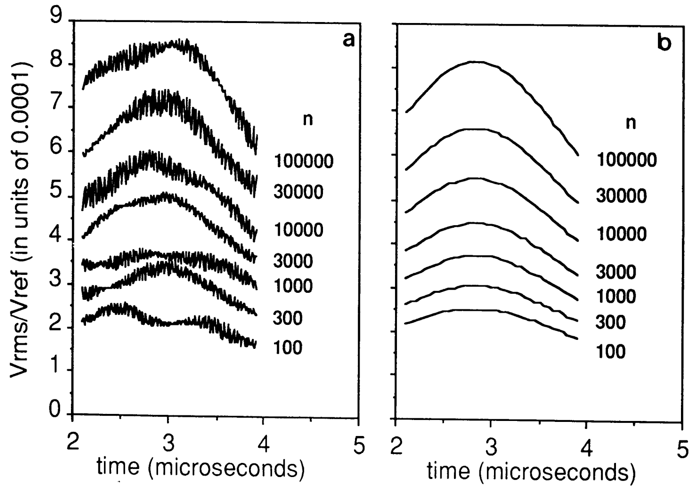

Fig. 5. RMS noise levels (a): Monte-Carlo Model. (b): Independent Scatterer Model.

respectively. The Gaussian probability function is also plotted using the observed mean and the variance of the voltage distributions in each case. For small-grained specimens, i.e., n = 100,000 grains per cubic cm of Fig. 6b., noise voltages are found to be distributed in a Gaussian manner. However, the distribution can be very non-Gaussian for large-grained specimens, i.e., for n = 100 grains per cubic cm of Fig. 6a. The ratio of the peak noise to rms noise averaged over a time window of interest can be used to track the approach to Gaussian behavior. Fig. 7 shows the Monte-Carlo model predictions of this average quantity for different grain densities (100 ensembles of grains at each density) for the toneburst equiaxial α-titanium inspection. The expected value of this ratio for a Gaussian distribution is shown by the solid line in Fig. 7. We observe that the ratio of peak noise to rms noise approaches the expected Gaussian level from above as the grain density increases.

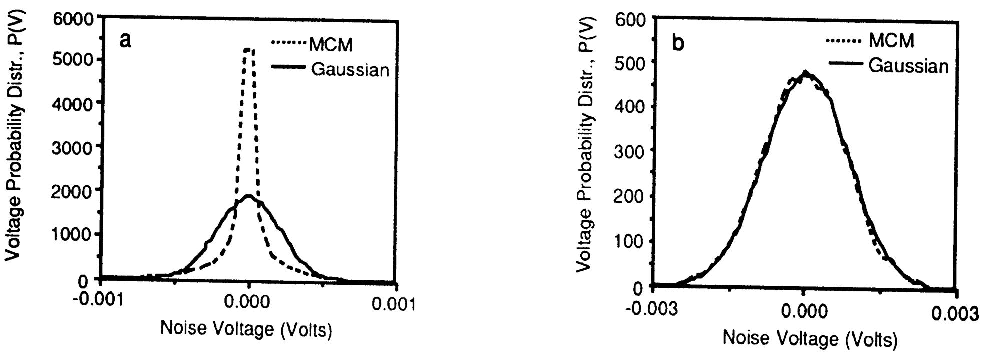

Fig. 6. Voltage distributions. (a): n = 100 grain/cm^3. (b): n = 100,000 grains/cm^3

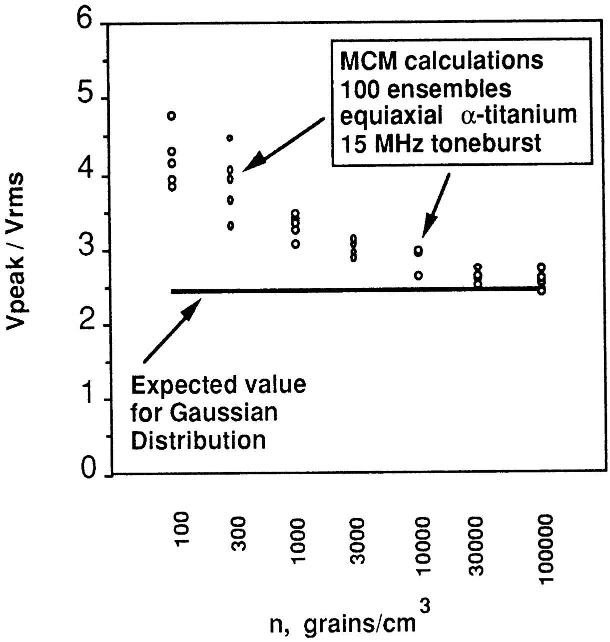

Fig. 7. Average peak noise to rms noise.

The Monte-Carlo noise model can also be used to provide waveforms for defect signals in the presence of noise. For example, simulated hard-alpha inclusions can be added to the cluster of grains. The predicted waveforms can then be used to test signal processing techniques for defect detection. The model can also be extended to include the effects of texture and grain elongation and may be integrated into a predictive detectability model for flaws in metals.

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REFERENCES

1. F. J. Margetan, T. A. Gray, and R. B. Thompson, Review of Progress in QNDE, 10B, D. O. Thompson and D. E. Chimenti, Eds., (Plenum Press, New York, 1991), p. 1721.
2. R. B. Thompson and T. A. Gray, J. Acoust. Soc. Am. 74(4): 1279-1290 (1983).
3. J. E. Gubernatis, E. Domany, J. A. Krumhansel, and M. Huberman, Laboratory of Atomic and Solid State Physics and Material Science Center, (Cornell University, Ithaca, New York, 1976), Report #2654.
4. R. B. Thompson and E. F. Lopes, J of Nondestr. Eval. 4(2): 107-123 (1984).
5. Yan Li and R. B. Thompson, J. Appl. Phys. 67(5): 2663-2665 (1990).
6. R. B. Thompson, J. F. Smith, S. S. Lee, and G. C. Johnson, Metal. Trans. 20A: 2431-2447 (1989).
7. B. A. Auld, (Wiley, New York, 1973), pp 73-86.
8. F. J. Margetan and R. B. Thompson, Review of Progress in QNDE, 11B, D. O. Thompson and D. E. Chimenti, Eds., (Plenum Press, New York, 1992), p. 1717.